

## 181. New Capabilities at the Center for Structural Molecular Biology at ORNL

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**Project Goals:** The Center for Structural Molecular Biology (CSMB) at Oak Ridge National Laboratory (ORNL) operates a small angle neutron scattering (SANS) instrument, called Bio-SANS, which is located at the High Flux Isotope Reactor. Bio-SANS is a 35m medium resolution SANS instrument that was specifically designed for biological studies and serves a vibrant user community of academic, industrial, and government users. Biological data from the SANS facility has the highest signal-to-noise ratio of any SANS instrument in this country. The Bio-Deuteration Laboratory (BDL) has significant strategic impact on neutron scattering at ORNL, providing benefits not just in higher quality and throughput of experiments but in extending the range, scale and complexity of biological problems that can be addressed. The CSMB complements other DOE OBER facilities for structural biology and supports studies of complex biological systems including biomolecular complexes, biomaterials, and biomass structure as part of the DOE Genomic Science Program.

The Bio-SANS instrument is ideally suited for studies of biomacromolecules including proteins, DNA/RNA, lipid membranes and other hierarchical complexes.<sup>1</sup> The recently upgraded Bio-SANS detector has count rate capabilities (>106 Hz) that enable utilization of the full potential of the high neutron flux from the cold source. In addition, we have developed a series of new sample environment capabilities that open untapped opportunities for the studies of biological systems using neutrons. These include a pressure cell to monitor chemical reactions in situ such as biomass pretreatment studies, a multi-position sample holder with rotational (tumbling) capability especially useful for studying suspensions, a humidity-controlled chamber critical for membrane studies and a flow cell for systems that partition to multiple phases (e.g., microemulsions) with additional capability of flowing one or two phases during measurement. Furthermore, we now can perform grazing-incident SANS in conjunction with a humidity chamber for studies of biomembranes and substrate-supported biosensors. The implementation of additional data reduction software, open source MantidPlot and streamlined operations together enhance the efficiency of the neutron scattering experiments for users. Recent upgrades in the BDL include a parallel bioreactor system that allows high-density cell growth with precise control and monitoring of dissolved oxygen, pH, agitation, and feeding rates and a second preparative scale bioreactor system for large-scale fermentations. Other new laboratory capabilities include a Rigaku single crystal diffractometer, two liquid handling robots for preparing crystallization screens, and a suite of incubators for temperature controlled protein crystallization.

### Reference

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*The Center for Structural Molecular Biology (CSMB) is supported by the Office of Biological and Environmental Research Project ERKP291, using facilities supported by the U. S. Department of Energy (DOE), managed by UT-Battelle, LLC under contract No. DE-AC05-00OR22725. Research at Oak Ridge*

*National Laboratory's High Flux Isotope Reactor and the Spallation Neutron Source is sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. DOE.*